



chain nodes :
 15 16 19 20 27 44 45
 ring nodes :
 1 2 3 4 5 6 7 8 9 10 11 12 13 14 28 29 30 31 32 33 34 35 36 37 38 39
 40 41
 chain bonds :
 2-19 7-15 10-16 12-27 19-20 27-29 34-44 37-45
 ring bonds :
 1-2 1-6 2-3 3-4 4-5 5-6 5-7 6-10 7-8 8-9 8-11 9-10 9-14 11-12 12-13 13-14 28-29
 28-33 29-30 30-31 31-32 32-33 32-34 33-37 34-35 35-36 35-38 36-37 36-41 38-39
 39-40 40-41
 exact/norm bonds :
 1-2 1-6 2-3 2-19 3-4 4-5 5-6 5-7 6-10 7-8 7-15 8-9 8-11 9-10 9-14 10-16 11-12
 12-13 12-27 13-14 19-20 27-29 34-44 37-45
 normalized bonds :
 28-29 28-33 29-30 30-31 31-32 32-33 32-34 33-37 34-35 35-36 35-38 36-37 36-41
 38-39 39-40 40-41

G1:Br,F,I,CH3,Et,n-Pr,s-Bu,CF2,CN,C,S,Si

G2:C,N

G3:C,I,F,NO2,S,N,Si,OH,SH,MeO,EtO

Match level :
 1:Atom 2:Atom 3:CLASS 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:Atom 11:Atom
 12:Atom 13:Atom 14:Atom 15:CLASS 16:CLASS 19:CLASS 20:CLASS 27:CLASS 28:CLASS 29:CLASS
 30:CLASS 31:Atom 32:Atom 33:Atom 34:Atom 35:Atom 36:Atom 37:Atom 38:Atom 39:Atom
 40:Atom 41:Atom 44:CLASS 45:CLASS